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1989 J. Phys. A: Math. Gen. 22 117

(http://iopscience.iop.org/0305-4470/22/1/018)

J. Phys. A: Math. Gen. **22** (1989) 117-128. Printed in the UK

Layering transitions in the chiral clock model: Bethe approximation

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Received 17 June 1988

Abstract. Interface phenomena, such as wetting and layering transitions of the three-state chiral clock model in three dimensions, are studied within the Bethe approximation. The Bethe approximation yields the correct sequence of first-order layering transitions. This is in contrast to the mean-field theory which is known to be qualitatively misleading for low temperatures. At higher temperatures the discontinuities of the order parameter at the layering transitions become exceedingly small so that the magnetisation profile appears to vary continuously across the interface. For finite values of the chiral field Δ the width of the interfacial layer is found to remain finite at the first-order bulk transition line. Critical wetting occurs only for $\Delta = 0$, i.e. for the symmetric three-state Potts model.

1. Introduction

At an interface between coexisting phases various structural phenomena can be observed. As the external parameters, most often the temperature, are varied phase transitions such as wetting, layering and roughening transitions may occur (for an overview see Sullivan and Telo da Gama (1986)). In this paper we study the behaviour of an interface in the three-state chiral clock (CC_3) model (Ostlund 1981, Huse 1981) in three dimensions. This layered spin model exhibits a modulated magnetisation along an axial direction whereas the magnetisation in the layers perpendicular to this direction is homogeneous. An interface between regions with different spin orientations may be introduced by fixing the spins in the top and bottom layers in two different states. We choose $n = 0$ in the bottom layer and $n = 2$ in the top layer (the three spin states will be labelled by $n = 0, 1, 2$). Depending on the temperature and on the value of the chiral field Δ the ensuing interface may be wetted with spins in the third state $n = 1$. It is known (Armitstead *et al* 1986) that at low temperatures this wetting occurs through a sequence of first-order layering transitions. At $\Delta = \frac{1}{4}$ an entire layer of $n = 1$ states intervenes between the $n = 0$ and $n = 2$ regions and the number of $n = 1$ layers increases in integer steps beyond $\Delta = \frac{1}{4}$. At higher temperatures one expects these first-order transitions to terminate at certain critical endpoints which accumulate at the roughening temperature (Wortis 1984, Pandit *et al* 1982, de Oliveira and Griffiths 1978). These phenomena cannot be investigated by the use of the mean-field (MF) approximation, since the MF theory of the CC_3 model is qualitatively misleading at low temperatures (Siegert and Everts 1985, Szpilka and Fisher 1986, 1987, Armitstead and Yeomans 1988). In particular it wrongly predicts that there should be only two layering transitions at low temperatures (Armitstead and Yeomans 1988). In previous work

0305-4470/89/010117+12$02.50

(Siegert and Everts 1987) it has been shown that the Bethe approximation, which is the first step beyond the MF approximation in the hierarchy of cluster variation methods, does not suffer from the deficiencies of the MF theory. It yields the correct bulk phase diagram of the CC_3 model in the low-temperature regime and it provides a detailed picture of the phase structure also at intermediate and high temperatures.

This paper is organised as follows. In the next section we describe the Bethe approximation of the model and show that this approximation comprises the low-temperature expansion of the original model. In § 3 we present and discuss the phase diagram obtained by a numerical evaluation of the Bethe approximation, in particular the differences of the phase transitions at low and high temperatures are elucidated. The behaviour of the interface close to the critical temperature of the bulk is studied in § 4 by a simplified approximation. For $\Delta = 0$ the thickness of the wet domain is found to diverge logarithmically, whereas it remains finite for $\Delta > 0$. The concluding § 5 contains a short summary of the paper.

2. The Bethe approximation and low-temperature expansions

The three-state chiral clock model on a three-dimensional layered lattice is defined by the Hamiltonian

$$H = -J_0 \sum_{\alpha} \sum_{\langle i,j \rangle} \cos \tfrac{2}{3}\pi (n_{i\alpha} - n_{j\alpha}) - J \sum_{\alpha} \sum_{i} \cos \tfrac{2}{3}\pi (n_{i\alpha} - n_{i\alpha+1} - \Delta) \qquad (2.1)$$

$$J_0, J > 0 \qquad n_{i\alpha} = 0, 1, 2.$$

Here the index α labels the two-dimensional layers and i, j count the lattice sites within a layer. Only nearest-neighbour interactions are included. The integer variables $n_{i\alpha}$ are connected with the local spin variables $\boldsymbol{S}_{i\alpha}$ by

$$\boldsymbol{S}_{i\alpha} = (\cos \tfrac{2}{3}\pi n_{i\alpha}, \sin \tfrac{2}{3}\pi n_{i\alpha}).$$

Within the layers these spins are coupled ferromagnetically, whereas in the axial direction the chiral field Δ favours an angle of $\frac{2}{3}\pi\Delta$ between two neighbouring spins. $\Delta = 0$ corresponds to the usual three-state Potts model. We consider the model in that part of the T-Δ parameter plane where the bulk state is ferromagnetic (Siegert and Everts 1987). An interface is introduced by fixing the spins in the first and the last layer in the states

$$n_{i1} = 0 \qquad n_{iN} = 2. \qquad (2.2)$$

By symmetry this interface is located in the middle of the system.

While in the MF approximation the free energy is assumed to depend only on the probabilities of finding single spins in one of the accessible states, Bethe's approximation works with a free energy function that depends on the probabilities of finding single spins and nearest-neighbour spin pairs in one of the accessible states. The entropy function of the CC_3 model in the Bethe approximation is (Siegert and Everts 1987)

$$S = \frac{k_B}{N} \sum_{\alpha=1}^{N} (5E_\alpha - 2Y_\alpha - U_\alpha) \qquad (2.3)$$

with

$$E_\alpha = \sum_{i=0}^{2} e_i(\alpha) \ln e_i(\alpha)$$

$$Y_\alpha = \sum_{i=0}^{2} y_i(\alpha) \ln y_i(\alpha) + 2 \sum_{i=3}^{5} y_i(\alpha) \ln y_i(\alpha)$$

$$U_\alpha = \sum_{i=0}^{8} u_i(\alpha) \ln u_i(\alpha).$$

Here $e_i(\alpha)$, $i = 0, 1, 2$, are the probabilities of finding a spin in the αth layer in one of the three possible states. $y_i(\alpha)$ and $u_i(\alpha)$ are the probabilities of finding a nearest-neighbour bond configuration in the αth layer and between the αth and the $(\alpha+1)$th layer as listed in table 1. The energy is given by

$$E = -\frac{1}{N} \sum_{\alpha=1}^{N} \left[2J_0 \left(\sum_{i=0}^{2} y_i(\alpha) - \sum_{i=3}^{5} y_i(\alpha) \right) + J \left(\cos \tfrac{2}{3}\pi\Delta \sum_{i=0}^{2} u_i(\alpha) \right.\right.$$
$$\left.\left. + \cos \tfrac{2}{3}\pi(1-\Delta) \sum_{i=3}^{5} u_i(\alpha) + \cos \tfrac{2}{3}\pi(1+\Delta) \sum_{i=6}^{8} u_i(\alpha) \right) \right] \tag{2.4}$$

and equations (2.3) and (2.4) yield the free energy of the CC_3 model in the Bethe approximation:

$$F(\{e\}, \{y\}, \{u\}) = E - TS. \tag{2.5}$$

The low-temperature expansions of spin models with a modulated magnetisation in one axial direction (Fisher and Selke 1981, Yeomans and Fisher 1984, Armitstead *et al* 1986) are expansions in powers of the Boltzmann weights of spin deviations from the ground state. To determine the phase boundaries of the layering transitions described in § 1 it suffices to take into account excited states in which the overturned spins are situated on axially connected chains with at most one protruding spin on the side (see figure 1) (Armitstead *et al* 1986). More precisely, to locate the phase boundary where the thickness of the intervening domain with $n_{i\alpha} = 1$ changes from l to $l+1$, one needs to consider excited states on chains of length l. For a comparison of the Bethe approximation with this direct low-temperature expansion one has to find out which excitations are treated correctly by the former. This question has, in a more general context, been investigated by Kurata *et al* (1953) and Hijmans and de Boer (1955). It follows from the work of these authors that in the expansion of the partition

Table 1. Probabilities for spin and spin pair states.

Spin state $n_{i\alpha}$	0	1	2						
Probability	$e_0(\alpha)$	$e_1(\alpha)$	$e_2(\alpha)$						
Spin pair state	0−0	1−1	2−2	0−1	0−2	1−2			
$n_{i\alpha} - \eta_{j\alpha}$				1−0	2−0	2−1			
Probability	$y_0(\alpha)$	$y_1(\alpha)$	$y_2(\alpha)$	$y_3(\alpha)$	$y_4(\alpha)$	$y_5(\alpha)$			
Spin pair state	0−0	1−1	2−2	0−1	1−2	2−0	0−2	1−0	2−1
$n_{i\alpha} - n_{i\alpha+1}$									
Probability	$u_0(\alpha)$	$u_1(\alpha)$	$u_2(\alpha)$	$u_3(\alpha)$	$u_4(\alpha)$	$u_5(\alpha)$	$u_6(\alpha)$	$u_7(\alpha)$	$u_8(\alpha)$

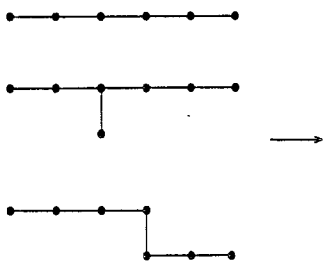

Figure 1. Spin-flip configurations which are taken into account in the low-temperature series. The arrow indicates the axial direction of the model.

function of the Bethe approximation the contributions of tree graphs, of which the above-mentioned chains are special examples, appear with the correct Boltzmann weights and with the proper multiplicities. Excitations corresponding to graphs that contain closed loops are not treated correctly by the Bethe approximation. Their contributions appear in the partition function with an improperly high order of the expansion parameter. Comparing the contributions of graphs of a given fixed length in the axial direction one sees that the contributions of graphs containing loops are of higher order in the expansion parameter than the contributions of the tree graphs. Thus, the error introduced by the improper treatment of the loop graphs in the Bethe approximation is of the same order as the error caused by neglecting them in the low-temperature expansion. Therefore the Bethe approximation must yield the correct low-temperature phase diagram. We checked this by a low-temperature expansion of the Bethe approximation up to third order (Siegert 1988).

3. Numerical results

In order to determine the stable magnetisation profile at the interface one has to minimise the free energy function (2.5) with the boundary conditions

$$\begin{aligned} e_0(1) &= 1 & e_1(1) &= e_2(1) = 0 \\ e_0(N) &= e_1(N) = 0 & e_2(N) &= 1. \end{aligned} \tag{3.1}$$

At higher temperatures where the ferromagnetic order is not perfect in the bulk these conditions are not well suited as they introduce strong boundary effects. It is more favourable to fix the modulus of the magnetisation at the boundaries to the value m_f of the bulk magnetisation of the ferromagnetic phase. This leads to the boundary conditions

$$\begin{aligned} e_0(1) &= \tfrac{1}{3}(1+2m_f) & e_1(1) &= e_2(1) = \tfrac{1}{3}(1-m_f) \\ e_0(N) &= e_1(N) = \tfrac{1}{3}(1-m_f) & e_2(N) &= \tfrac{1}{3}(1+2m_f). \end{aligned} \tag{3.2}$$

m_f must be determined separately from the equilibrium conditions of the bulk system (see Siegert and Everts 1987). By the use of the conditions (3.2) instead of (3.1) boundary effects are considerably reduced (figure 2).

Interface phenomena are most conveniently studied by considering excess quantities that characterise the properties of the interface. The interfacial free energy is defined as

$$\Delta F = F - F_f \tag{3.3}$$

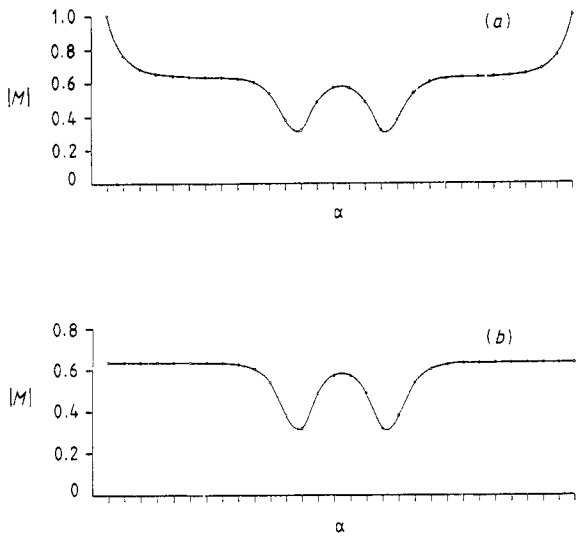

Figure 2. Modulus of the magnetisation, (*a*) for the boundary conditions (3.1), (*b*) for the boundary conditions (3.2). $T/J = 2.5$, $\Delta = 0.32$.

where F is the free energy (2.6) of a system containing an interface and F_f is the free energy of a system without an interface, i.e. F_f is the free energy of the ferromagnetic bulk phase. As an order parameter that reflects the phase transitions at the interface we introduce the excess of $n = 1$ states at the interface:

$$p_1 = \sum_{\alpha=1}^{N} [e_1(\alpha) - e_{1f}]. \tag{3.4}$$

Here

$$e_{1f} = \tfrac{1}{3}(1 - m_f)$$

is the probability of finding $n = 1$ states in the bulk. For $T = 0$, p_1 takes only integer values, $p_1 = 0, 1, 2, \ldots$, corresponding to the number of layers with $e_1(\alpha) = 1$.

The minimisation of the free energies (2.5) and (3.3) is achieved by the same numerical iteration procedure as has previously been applied in the case of the bulk problem (Siegert and Everts 1987). Depending on the initial conditions of the iteration procedure different interfacial configurations are obtained; the true stable configuration at a given point in the T-Δ plane corresponds to the absolute minimum of the free energy. Depending on the temperature we choose a system length between $N = 50$ and $N = 100$ layers. For $N \geqslant 90$ no dependence of the excess free energy ΔF and of the order parameter p_1 on the system length N was observed for any temperature below the bulk transition temperature $T_b(\Delta)$. The resulting interface phase diagram is shown in figure 3 (in our numerical calculations we have always set $J_0 = J$). At all the phase boundaries the order parameter p_1 jumps by a finite amount and the transitions are of first order. For low temperatures $T/J \leqslant 1.7$ the transition lines $T_{l,l+1}(\Delta)$ behave as predicted by the low-temperature expansion. The jumps Δp_1 of the order parameter at the phase boundaries are almost unity (figure 4(*a*)). For higher temperatures the situation changes drastically: the transition lines $T_{l,l+1}(\Delta)$ bend back towards small Δ as the temperature increases, yielding a wetting transition even at $\Delta = 0$. Simultaneously the jump Δp_1 of the order parameter decreases to very small values (figures 4(*b*, *c*)),

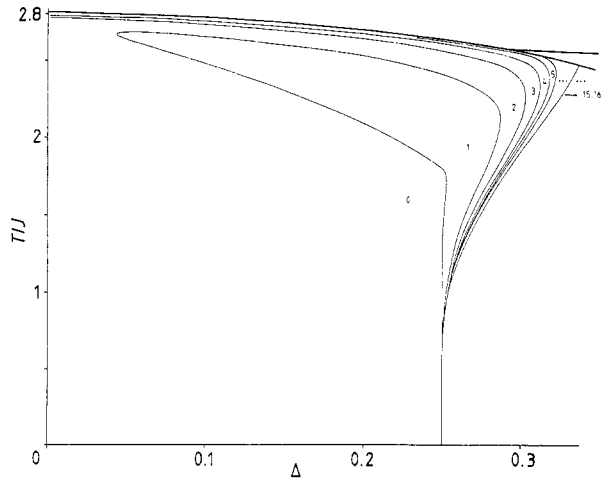

Figure 3. Interfacial phase diagram of the CC_3 model in the Bethe approximation. The phases are characterised by the values of their order parameter p_1 at $T = 0$. The full curves display phase transitions of the bulk.

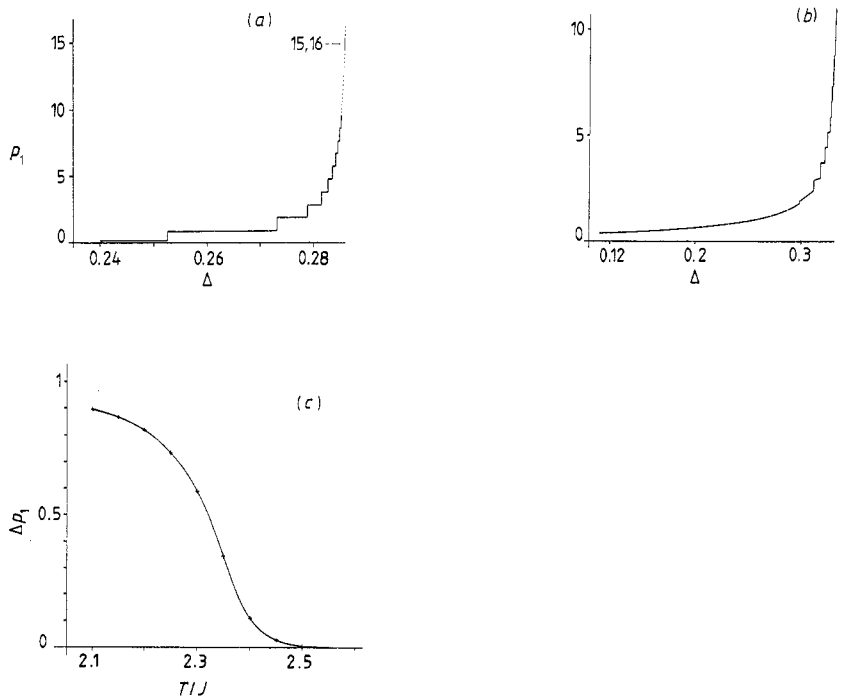

Figure 4. Order parameter $p_1(a)$ at low temperatures ($T = 1.7J$), (b) at higher temperatures ($T = 2.4J$); (c) jump Δp_1 of the order parameter at the 2, 3 phase boundary.

e.g. $\Delta p_1 = 8.66 \times 10^{-4}$ at $T_{0,1} = 2.4J$, $\Delta_{0,1} = 0.126$ and $\Delta p_1 = 8.70 \times 10^{-3}$ at $T_{1,2} = 2.4J$, $\Delta_{1,2} = 0.256$, which are not resolved in figure 4(*b*). The phase transition appears to be quasicontinuous. The centre of the interface is always localised either in the middle between two lattice layers (l even) or at a layer (l odd). This is in contradiction to the expectation (Pandit *et al* 1982) that the first-order layering transitions terminate at critical endpoints that accumulate at the roughening temperature where the interface is delocalised. We suspect that a true roughening transition cannot be detected within the Bethe approximation. Probably, the small jumps in the order parameter that define the upper decreasing branches of the transition lines are artefacts of the Bethe approximation, i.e. the transition lines should end at points $T_{l,l+1}$ where their slopes are still positive. In particular the closing of the $T_{0,1}(\Delta)$ transition line for small values of Δ in figure 3 is presumably unphysical. Nevertheless, the growing thickness of the intervening $n = 1$ layers with increasing temperature, which is reflected by the negative slopes of the transition lines at higher temperatures, is in keeping with the notion that the walls of the $n = 1$ layers repel each other due to their roughness.

Since the jumps of p_1 that reflect a deficiency of the Bethe approximation are exceedingly small whenever they occur in the vicinity of the bulk transition temperature $T_b(\Delta)$, e.g. we find $\Delta p_1 = 7.75 \times 10^{-10}$, $p_1 = 0.781$ at $T_{2,3}(\Delta = 0) = 2.782J$, we expect the approximation to be useful for an analysis of the wetting layer in the vicinity of $T_b(\Delta)$. Figure 5 shows a typical magnetisation profile for a temperature close to $T_b(\Delta = 0)$. A paramagnetic layer intrudes between the $n = 0$ and the $n = 2$ domains. From the numerical analysis we find that the length Λ of this paramagnetic layer diverges logarithmically as T approaches $T_b(\Delta = 0)$, while the modulus of the magnetisation at the centre of the layer decreases as $t^{1/2}$, $t = 1 - T/T_b(\Delta = 0)$, and the order parameter p_1 is roughly proportional to Λ, $p_1 \simeq \frac{1}{3} m_f \Lambda$. Similar critical properties of an interface have been observed in several other models (Widom 1978, Lajzerowicz 1981, Lipowsky 1982). For $\Delta \neq 0$ the behaviour of the interface is different. Figure 6 shows a section of the phase diagram around $\Delta = 0.3$. For $l \geqslant 5$ the phase boundaries $T_{l,l+1}(\Delta)$ intersect the first-order transition line between the ferromagnetic and the modulated phases of the bulk at certain points $T^{(a)}_{l,l+1}$, $\Delta^{(a)}_{l,l+1}$ and re-enter the ferromagnetic region of the bulk phase diagram at points $T^{(b)}_{l,l+1}$, $\Delta^{(b)}_{l,l+1}$. The order parameter p_1 is finite at the re-entry points corresponding to a finite thickness of the wetting layer for $\Delta \neq 0$. However, the values $\Delta^{(b)}_{l,l+1}$ decrease to zero as l increases; $p_1(\Delta^{(b)}_{l,l+1})$ diverges simultaneously, thus matching the critical behaviour at $\Delta = 0$. Furthermore, as shown in figure 6, the point $\Delta^{(a)}_{5,6}$, $T^{(a)}_{5,6}$ lies in the region of stability of the modulated bulk phases with wavenumbers $q = \frac{2}{15}\pi$, $\frac{2}{18}\pi$. These bulk phases are periodic sequences of five or

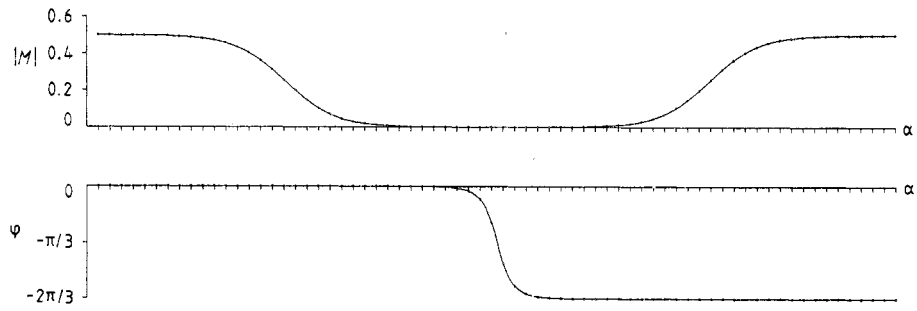

Figure 5. Modulus $|M|$ and phase φ of the magnetisation at the reduced temperature $t \simeq 4.5 \times 10^{-9}$. $T/J = 2.819\,2973$, $\Delta = 0$, $p_1 = 6.138$.

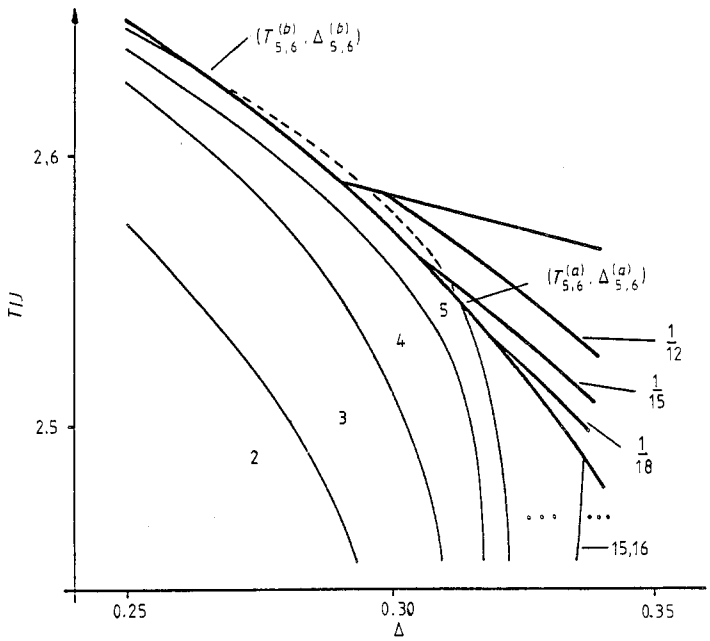

Figure 6. Section of the phase diagram showing the two intersections of the 5, 6 phase boundary with the transition line of the ferromagnetic bulk phase.

six consecutive layers of (predominantly) identical spins. The thickness l of the interfacial layer and the structure of the bulk phase are thus seen to match on the bulk transition line.

4. Simplified model for the interface

In the vicinity of the transition temperature of the bulk $T_b(\Delta)$ the properties of the interfacial layer, in particular the critical properties at $\Delta = 0$, should be obtainable from the Landau expansion of the MF free energy ($m_1(\alpha)$, $m_2(\alpha)$ are the components of the layer magnetisation)

$$
\begin{aligned}
-\beta F_{MF} = \frac{1}{N}\sum_{\alpha=1}^{N} \{&(2K_0-1)(m_1^2(\alpha)+m_2^2(\alpha)) \\
&+\tfrac{1}{2}Km_1(\alpha)[\cos\tfrac{2}{3}\pi\Delta(m_1(\alpha+1)+m_1(\alpha-1)) \\
&+\sin\tfrac{2}{3}\pi\Delta(m_2(\alpha+1)-m_2(\alpha-1))] \\
&+\tfrac{1}{2}Km_2(\alpha)[\cos\tfrac{2}{3}\pi\Delta(m_2(\alpha+1)+m_2(\alpha-1)) \\
&-\sin\tfrac{2}{3}\pi\Delta(m_1(\alpha+1)-m_1(\alpha-1))] \\
&+\tfrac{1}{3}(m_1^3(\alpha)-3m_1(\alpha)m_2^2(\alpha))-\tfrac{1}{2}(m_1^2(\alpha)+m_2^2(\alpha))^2+O(m_{1,2}^5(\alpha))\}. \qquad (4.1)
\end{aligned}
$$

Instead of F_{MF} one could have expanded the Bethe approximation of the free energy. This would have resulted in a more complicated expression than (4.1). Since the jump in the bulk magnetisation at $T_b(\Delta)$ is approximately 0.5 in both approximations either

of the expansions will only yield qualitative results. We therefore regard the simpler expression (4.1) as a simplified model which we expect to provide a qualitative correct description of the properties of the interface for $T \leqslant T_b(\Delta)$.

From (4.1) one finds a first-order bulk phase transition at

$$T_b(\Delta) = \tfrac{18}{17}(2J_0 + J_1) \qquad J_1 = J\cos\tfrac{2}{3}\pi\Delta. \tag{4.2}$$

The ferromagnetic bulk magnetisation is given by

$$m_f = \tfrac{1}{4} + (2K_0 + K_1 - \tfrac{15}{16})^{1/2} \qquad K_i = J_i/T \qquad i = 0, 1. \tag{4.3}$$

It has a discontinuity at $T_b(\Delta)$ of $\Delta m_f = \frac{1}{3}$. Using the definitions

$$m_i(\alpha+1) - 2m_i(\alpha) + m_i(\alpha-1) =: m_i''(\alpha)$$

$$m_i(\alpha+1) - m_i(\alpha-1) =: 2m_i'(\alpha) \qquad i = 1, 2$$

we take the contiuum limit of (4.1) and arrive at ($K = J/T$)

$$\begin{aligned} -\beta F = \frac{1}{2L}\int_{-L}^{L} \mathrm{d}z \{ & (2K_0 + K_1 - 1)(m_1^2(z) + m_2^2(z)) + \tfrac{1}{2}K_1(m_1(z)m_1''(z) + m_2(z)m_2''(z)) \\ & + K\sin\tfrac{2}{3}\pi\Delta(m_1(z)m_2'(z) - m_2(z)m_1'(z)) \\ & + \tfrac{1}{3}(m_1^3(z) - 3m_1(z)m_2^2(z)) - \tfrac{1}{2}(m_1^2(z) + m_2^2(z))^2 \}. \end{aligned} \tag{4.4}$$

The components of the magnetisation are determined by the Euler-Lagrange equations to the functional (4.4):

$$\begin{aligned} m_1''(z) + 2\tan\tfrac{2}{3}\pi\Delta m_2'(z) + \frac{1}{K_1}[& 2(2K_0 + K_1 - 1)m_1(z) + m_1^2(z) - m_2^2(z) \\ & - 2m_1(z)(m_1^2(z) + m_2^2(z))] = 0 \end{aligned} \tag{4.5a}$$

$$\begin{aligned} m_2''(z) - 2\tan\tfrac{2}{3}\pi\Delta m_1'(z) + \frac{1}{K_1}[& 2(2K_0 + K_1 - 1)m_2(z) - 2m_1(z)m_2(z) \\ & - 2m_2(z)(m_1^2(z) + m_2^2(z))] = 0. \end{aligned} \tag{4.5b}$$

For $\Delta = 0$ we expect to find a solution of (4.5*a*, *b*) that agrees qualitatively with the profiles shown in figure 5, i.e. for $-L \leqslant z \leqslant 0$ either $m_1(z) \gg |m_2(z)|$ or $m_1(z), |m_2(z)| \ll 1$ should be fulfilled at least for sufficiently small values of the reduced temperature $t = (T_b(\Delta = 0) - T)/T$. Equations (4.5) may thus be simplified to

$$m_1''(z) + \frac{1}{K}[2(2K_0 + K - 1)m_1(z) + m_1^2(z) - 2m_1^3(z)] = 0 \tag{4.6a}$$

$$m_2''(z) + \frac{2}{K}(2K_0 + K - 1)m_2(z) = 0. \tag{4.6b}$$

These are solved by ($z \leqslant 0$)

$$m_1(z) = \frac{am_f\sinh(-\kappa z + c) - \mu}{1 + a\sinh(-\kappa z + c)} \tag{4.7a}$$

$$m_2(z) = a_2\,\mathrm{e}^{\eta z} \tag{4.7b}$$

where

$$a^2 = \frac{3m_f - 1}{(6m_f - 1)^2} \tag{4.8a}$$

$$\mu = 2m_f \frac{3m_f - 1}{6m_f - 1} \tag{4.8b}$$

$$\kappa = \left(\frac{m_f}{K}(4m_f - 1)\right)^{1/2} \tag{4.8c}$$

$$\eta = \left(\frac{1}{K}(1 - 2m_f)\right)^{1/2}. \tag{4.8d}$$

The constants c and a_2 are determined by the conditions $m'(z=0)=0$, $\varphi(z=0)=-\frac{1}{3}\pi$ which the modulus m and the phase φ of the magnetisation must fulfil by symmetry:

$$\sinh c = \frac{1}{2\sqrt{2}} + \frac{135}{64}(3m_f - 1)^{1/2} + O(t)$$

$$a_2 = -\sqrt{3}\,\frac{a m_f \sinh c - \mu}{1 + a \sinh c}.$$

The maximum error of the functions (4.7) compared with numerical solutions of the differential equations (4.5) at $\Delta = 0$ is about 1% at $t \simeq 10^{-7}$. From (4.3) and (4.8*a*, *b*) it follows that $a \sim t^{1/2}$ and $\mu \sim t$ so that $a_2 \sim t^{1/2}$ (note that $3m_f - 1 \sim t$). Hence the modulus of the magnetisation $m(z)$ varies as $t^{1/2}$ for $|z| \ll L$, while the slope of the phase $\varphi(z) = \tan^{-1}(m_2(z)/m_1(z))$ tends to a constant at $T = T_b(\Delta = 0)$:

$$\varphi'(z=0) = -\left(\frac{T_b(\Delta=0)}{3J}\right)^{1/2} \qquad T = T_b(\Delta = 0).$$

The point of inflection z_0 of $m(z)$, $m''(z_0) = 0$, may be used as a measure of the length Λ of the paramagnetic domain:

$$\Lambda = -2z_0 \simeq \frac{2}{\kappa}(\ln 2/a - c - \tfrac{7}{4}a^2).$$

This behaviour of the interface at $\Delta = 0$ is the same as found in other models (Widom 1978, Lajzerowicz 1981, Lipowsky 1982).

For $\Delta \neq 0$ we are not able to find an acceptable approximate analytic solution for equations (4.6). The numerical solutions of these equations (figure 7) show the same

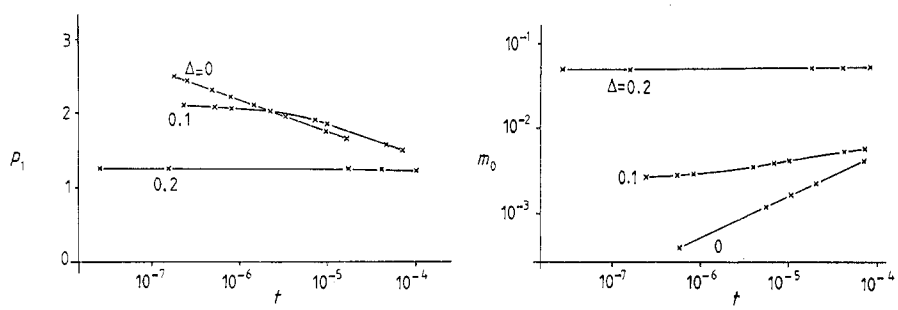

Figure 7. Order parameter p_1 and modulus $m_0 = m(z=0)$ of the magnetisation for various values of Δ.

behaviour as found within the Bethe approximation. In contrast to the case $\Delta = 0$ the magnetisation $m(z=0)$ and the order parameter $p_1 \sim \Lambda$ tend to finite values as T approaches $T_b(\Delta)$. For small values of Δ we observe an antichiral ordering, $\varphi(z=0) = -\frac{1}{3}\pi$, whereas at larger values of Δ a chiral order ($\varphi(z=0) = \frac{2}{3}\pi$) is present. Thus, for $T \simeq T_b(\Delta)$ the simple model defined by the free energy functional (4.1) yields qualitatively the same results as the numerical treatment of the Bethe approximation.

5. Summary

In this paper the Bethe approximation has been used to study interface properties of the three-state chiral clock model in three dimensions. We have shown that the Bethe approximation yields the exact low-temperature phase diagram. The arguments that lead to this conclusion apply not only to the CC_3 model but to any layered model for which only the excitations corresponding to tree graphs are needed in the determination of the low-temperature phase diagram. For higher temperatures the behaviour of the interface deviates considerably from that at low temperatures. The jumps of the order parameter at the first-order layering transitions decrease to very small values and the transitions appear to be quasicontinuous. Nevertheless, it is found that these transitions remain first order at all temperatures. Critical endpoints that would indicate a roughening transition has not been found. We suspect that this is a deficiency of the Bethe approximation. An intuitive picture of the correct phase diagram is displayed in figure 8. The roughening temperature $T_R(\Delta)$ may be slightly Δ dependent, but it will be of

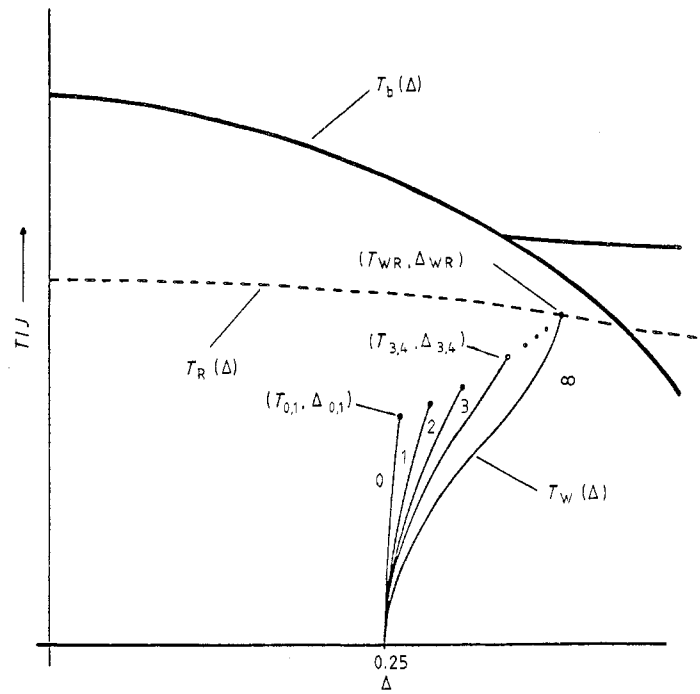

Figure 8. Interfacial phase diagram of the CC_3 model including roughening effects (schematic).

the same magnitude as the critical temperature of the two-dimensional three-state Potts model. $T_R(\Delta)$ will therefore intersect the wetting transition line $T_W(\Delta)$ at a point T_{WR}, Δ_{WR}. All first-order layering transition lines terminate at critical endpoints $T_{l,l+1}$, $\Delta_{l,l+1}$ which accumulate at T_{WR}, Δ_{WR}. This resembles the picture found for multilayer adsorption in a lattice gas model (de Oliviera and Griffiths 1978, Pandit *et al* 1982). The thickness of the wetting layer at the bulk transition temperature $T_b(\Delta)$ remains finite for all finite values of Δ, whereas it diverges logarithmically for $\Delta = 0$, i.e. for the symmetric three-state Potts model.

Acknowledgments

We should like to thank J M Yeomans and W Selke for interesting discussions. Financial support from the Bundesministerium für Forschung und Technologie is gratefully acknowledged. The numerical calculations were performed at Regionales Rechenzentrum für Niedersachsen, Hannover.

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